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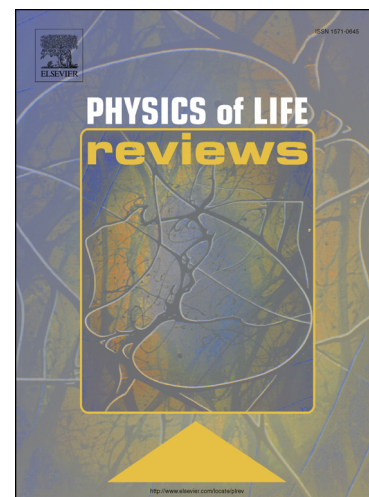
Ligand diffusion in proteins via enhanced sampling in molecular dynamics

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Highlights

- The process of ligand recognition by proteins is fundamental in the physics of living organisms.
- The complex topology of protein channels and the transient nature of the ligand passage pose difficulties in the modeling of the ligand entry/escape pathways by canonical molecular dynamics simulations.
- The need for identifying the ligand egress pathways and understanding how ligands migrate through protein tunnels has spurred the development of several methodological approaches.

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